Plane Couette Flow Computations by TRMC and MFS Methods

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Abstract. A new class of schemes of the DSMC type for computing near-continuum flows has been recently suggested: the time-relaxed Monte Carlo (TRMC) methods. An important step preceding the wide use of these schemes is their validation by classical homogeneous and one-dimensional problems of gas dynamics. For this purpose, a plane Couette flow is considered in the present paper. A comparison of TRMC results with the data obtained by time-proved schemes of the DSMC method (here we used the Majorant Frequency Scheme) in a wide range of Knudsen numbers and for different values of wall velocity is presented.

INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method [1] is the best developed and powerful tool of simulation of multidimensional gas flows at the kinetic level. The main drawback of this method is the high computational cost in computing near-continuum flows (with Knudsen numbers $\mathrm{Kn} < 0.01$). Therefore, it is of interest to develop new, numerically effective schemes of the DSMC method.

A new class of promising schemes of the DSMC method for computing near-continuum flows has been recently suggested [2] : the time-relaxed Monte Carlo (TRMC) methods. An important step preceding the wide use of these schemes is their validation by classical homogeneous and one-dimensional problems of gas dynamics. For this purpose, a plane Couette flow is considered in the present paper. The plane Couette flow is a simple one-dimensional flow where typical features of multidimensional gas flows are manifested: nonuniform distribution of the gas in space, velocity slip and temperature jump near the surface of the plates, strong influence of viscosity, and heat transfer in the gas.

Exact duplication of these effects in the course of simulation indicates whether the method can yield a solution corresponding to the solution of the Boltzmann equation. For these reasons, the plane Couette flow is fairly suitable for validation of new schemes of the DSMC method, such as TRMC schemes.

The goal of the present study is to compare TRMC results with the data obtained by time-proved schemes (Majorant Frequency Scheme (MFS)) of the DSMC method in a wide range of Knudsen numbers for different values of dimensionless wall velocity. In analyzing the modeling results, special attention will be paid to high-order moments of the distribution function (such as the heat-flux vector), which offer an explicit demonstration of the simulation quality, in contrast to low-order moments (such as density and velocity).

SPATIALLY INHOMOGENEOUS BOLTZMANN EQUATION

Let us consider the Boltzmann equation, which is 1D in space and 3D in velocity. Then the equation reads

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} = \frac{1}{\mathrm{Kn}} Q(f, f)$$

where the equation is written in dimensionless form and Kn denotes the Knudsen number. If the space is divided into a certain number of cells, and the time is divided into discrete intervals of size Δt, then it is possible to solve the Boltzmann equation by a splitting method. First, the collisional step is performed in each cell, as in the spatially

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homogeneous case, then the convection step is computed for a free flow $x_i = x_i + v_{xi}\Delta t$ over all particles. If the particle crosses the solid surfaces then the particle-surface interaction is performed (reflection of the particle with a new velocity). The convection step is performed in the same manner for both schemes, whereas the implementation of the collisional step is different in MFS and TRMC schemes.

MAJORANT FREQUENCY SCHEMES

The DSMC method is traditionally considered as a method of computer simulation of the behavior of a great number of model gas molecules. Each simulated particle is then regarded as representing an appropriate number F_n of real molecules. The state of each model particle is characterized by its coordinate r and velocity v. The evolution of a system of N model particles can be represented as a jump-like motion of a point $\{\bar{R},\bar{V}\} = \{r_1, v_1, ..., r_N, v_N\}$ in the $6N$-dimensional phase space. The DSMC method can be then treated as computer simulation of the $6N$-dimensional random jump-like process. For such a simulation, we represent the trajectory of the random process from the initial trajectory point of the random process $(t_0, \bar{R}_0, \bar{V}_0)$, as a transition in time between subsequent collisions (free motion) from the state $(t_0, R_0, \bar{V}_0)$ to the state $(t_1, R_1, \bar{V}_0)$, and the changes in particle velocities after collisions, i.e., the transition from the state $(t_1, R_1, \bar{V}_0)$ to $(t_1, R_1, \bar{V}_1)$. MFS construction can be illustrated by a simple case of a spatially homogeneous gas flow. For a spatially homogeneous rarefied gas flow case, there is no dependence on spatial coordinates $\bar{R}$, and the process can be simulated only in a $3N$-dimensional space of velocities $\{\bar{V}\}$.

The so-called "master" kinetic equations (MKE) [3], [4], [5] describe the behavior of an N-particle gas model with binary collisions. These linear MKEs transform to the nonlinear Boltzmann equation as $N \to \infty$ and molecular chaos conditions are satisfied (see, e.g., [7]). It is natural to use directly these equations for constructing numerical schemes of the DSMC method.

Using a function w – the probability density of the transition of a pair of particles from (v_i', v_j') to (v_i, v_j) – Kac's MKE in a spatially homogeneous rarefied gas flow case is written as

$$\frac{\partial}{\partial t} f_N(t,\bar{V}) + \nu(\bar{V}) f_N(t,\bar{V}) = \frac{n}{N} \sum_{i<j} \int f_N(t,\bar{V}_{ij}') w(v_i', v_j' \to v_i, v_j) dv_i' dv_j',$$

where the sum over $i<j$ means summation over $N(N-1)/2$ collision pairs, $\nu(\bar{V})$ is the total collision frequency,

$$\nu(\bar{V}) = \frac{n}{N} \sum_{i<j} \sigma_t(g_{ij}) g_{ij} < \infty,$$

g is the relative collision velocity, and $\sigma_t(g_{ij})$ is the total collision cross section. By introducing the majorant collision frequency [6]

$$\nu_m = \frac{N(N-1)}{2} [g\sigma_t(g)]_{max} \geq \nu(\bar{V})$$

, summation over $N(N-1)/2$ collision pairs can be avoided, and MKE can be transformed to be suitable for constructing a random process that describes the behavior of the N-particle gas model with computational time linearly depending on the number of modeling molecules N.

For a spatially homogeneous case, the time of the next collision t_1 has a probability density distribution $\nu_m \exp\{-\nu_m(t_1 - t_0)\}$. For the transition $(t_1, \bar{V}_0) \to (t_1, \bar{V}_1)$, a collisional pair (i, j) is uniformly chosen from $N(N-1)/2$ pairs. A real collision occurs with a probability $P = \frac{g_{ij}' \sigma_t(g_{ij}')}{[g\sigma_t(g)]_{max}}$, and with a probability $(1-P)$ the velocities will not change, i.e., a fictitious collision occurs.

For the spatially inhomogeneous case, such a procedure is performed in each collisional cell, and a detailed description of MFS derivation in the case of a spatially inhomogeneous gas flow can be found in [8].

TIME-RELAXED MONTE CARLO METHODS

Time-Relaxed schemes are based on a formal expansion of the solution of the Boltzmann equation, called Wild sum Expansion ([9, 2]), and on its subsequent probabilistic interpretation. Note that this probabilistic interpretation holds uniformly for any time step.

From the Wild sum expansion of the Boltzmann equation, the following class of numerical schemes is obtained:

$$f^{n+1}(v) = (1-\tau)\sum_{k=0}^{m} \tau^k f_k^n(v) + \tau^{m+1} M(v).$$

Here, $f^n \approx f(n\Delta t)$, Δt is a small time interval, and $\tau = 1 - e^{-\mu \Delta t/\mathrm{Kn}}$

Such methods preserve the moments and are *asymptotically preserving*, i.e., in the limit $\mathrm{Kn} \to 0$, the function is projected into a Maxwellian function. The time accuracy depends on the level of truncation m.

A generalization of the above-given schemes (generalized TRMC) can be written as

$$f^{n+1}(v) = \sum_{k=0}^{m} A_k f_k^n(v) + A_{m+1} M(v).$$

where the weights $A_k = A_k(\tau)$ are nonnegative functions satisfying some conservation consistency and the asymptotic preservation property. A more detailed description can be found in [2].

TRMC schemes are a direct consequence of the probabilistic interpretation of the truncated expansion of the Wild sum expansion. Here we illustrate the third-order TR method. Even if we do not consider a spatially homogeneous problem, we can continue to assume that f can be normalized to unity, so that it has the meaning of the probability density.

We recall ([2]) for the case of the first- and second-order TR schemes. Third-order TR scheme (TRMC3): For $m = 3$, the generalized TR schemes yield

$$f^{n+1} = A_0 f^n + A_1 f_1 + A_2 f_2 + A_3 f_3 + A_4 M$$

Since A_k, $k = 0,1,2,3,4$, are nonnegative numbers that are summed up to give unity, they are probabilities ([2]). Furthermore, $f_1 = P(f^n, f^n)/\mu$ is also a probability density. The probabilistic interpretation of the equation given above is as follows.

A particle extracted from f^n

- does not collide with a probability A_0, (i.e., it is sampled from f^n);
- collides with another particle extracted from f^n with a probability A_1 (i.e., it is sampled from the function f_1);
- collides with another particle extracted from f_1 (i.e., with a particle involved in just one collision before) with a probability A_2 (i.e., it is sampled from the function f_2);
- collides the first time with a particle sampled by f^n and the second time with a particle extracted by f_1 (i.e., with a particle already involved in one collision) with a probability $\frac{1}{3}A_3$ (i.e., the particle is sampled from the function $\frac{P(f_1,f_1)}{\mu}$;
- collides with a particle extracted from f_2 (i.e., with a particle involved in exactly two collisions) with a probability $\frac{2}{3}A_3$ (i.e., the particle is sampled from the function $\frac{P(f_2,f_0)}{\mu}$;
- is replaced by a particle sampled from the Maxwellian function with a probability A_4.

Remark. In this formulation, the probabilistic interpretation holds uniformly in $\mu\Delta t$, in contrast to schemes based on different time discretization of the equation, which require $\mu\Delta t < c$, for some suitable $c > 0$. Furthermore, as $\mu\Delta t \to \infty$, the distribution at the time $n+1$ is sampled from the Maxwellian function. In a spatially inhomogeneous case, this would be equivalent to a particle method for the Euler equations. In all our numerical tests, we use TRMC3 (i.e. $m = 3$).

NUMERICAL RESULTS

The formulation of the plane Couette flow problem is as follows. Let us consider two infinite parallel plates (L is the distance between the plates). The area between the plates is filled by a monatomic gas with an average density n_0. The diffuse reflection law is set at the surface of the plates. The plates have equal temperatures T_w. The molecular weight is m, the total cross section is σ, and the molecules collide according to the Hard Sphere model. The left plate is stationary, and the right plate moves in the y direction (in its own plane) with a velocity V_w. The mean free path is

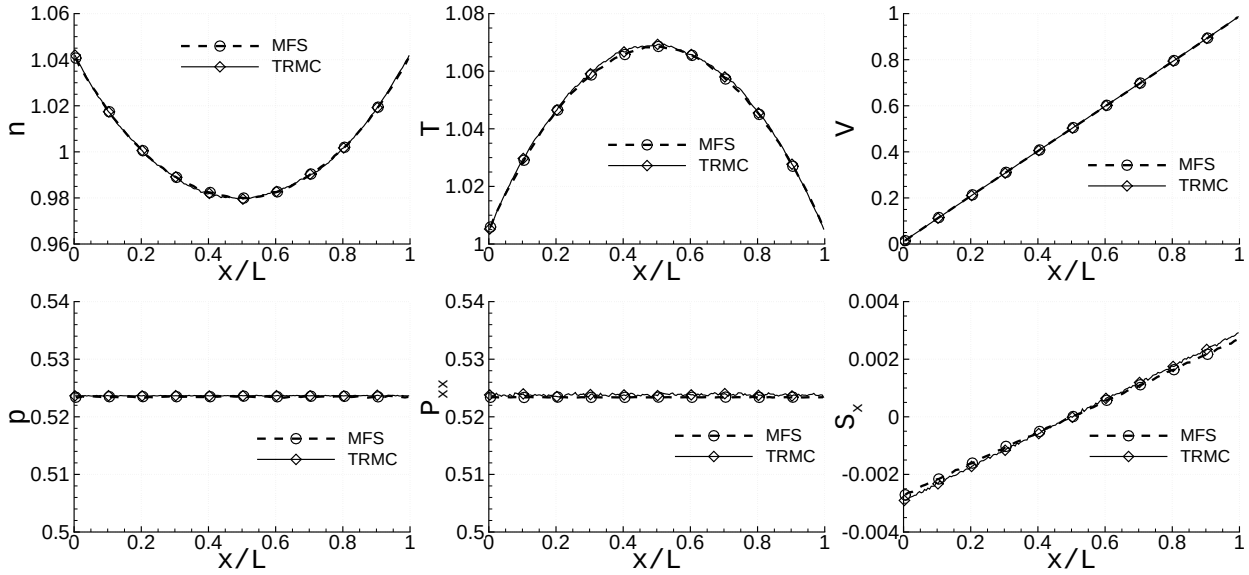

FIGURE 1. Knudsen number Kn $= 0.01$, plate velocity $S = 1$

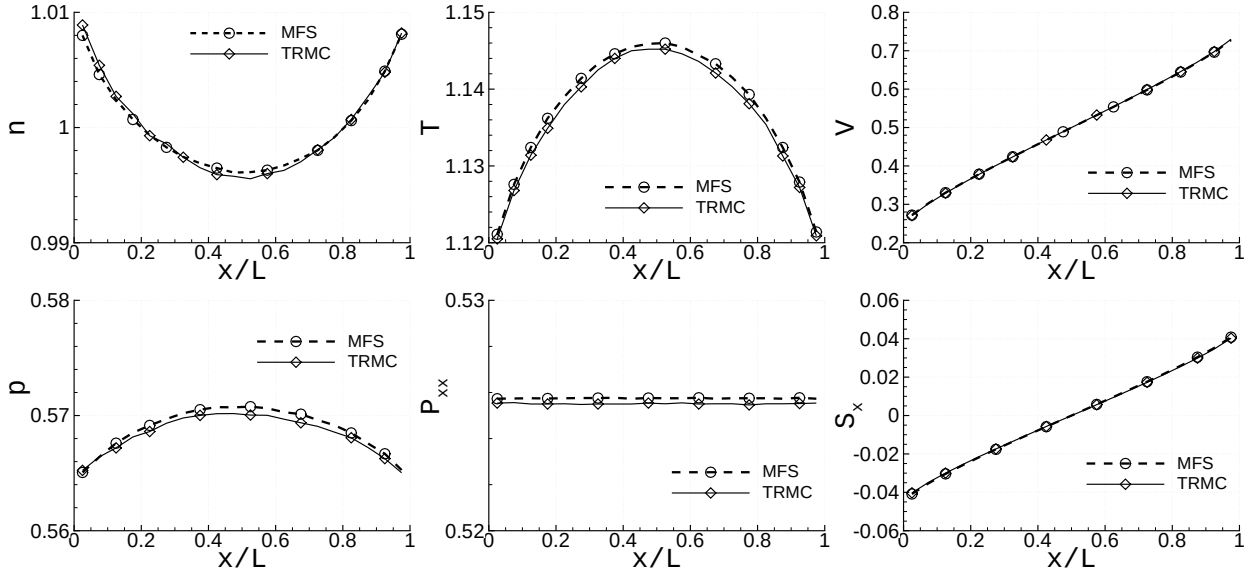

FIGURE 2. Knudsen number Kn $= 1$, plate velocity $S = 1$

$\lambda_0 = 1/(\sqrt{2}n_0\sigma)$, and the Knudsen number is Kn $= \lambda_0/L$. The parameter S is the right wall velocity V_w normalized to the most probable thermal velocity $V_t = \sqrt{2kT_w/m}$: $S = V_w/V_t$.

We considered four cases summarized in the table below.

Case	Kn	S	N cells	N part./cell
1	0.01	1.0	200	100
2	1.0	1.0	20	100
3	0.01	5.0	200	100
4	1.0	5.0	20	100

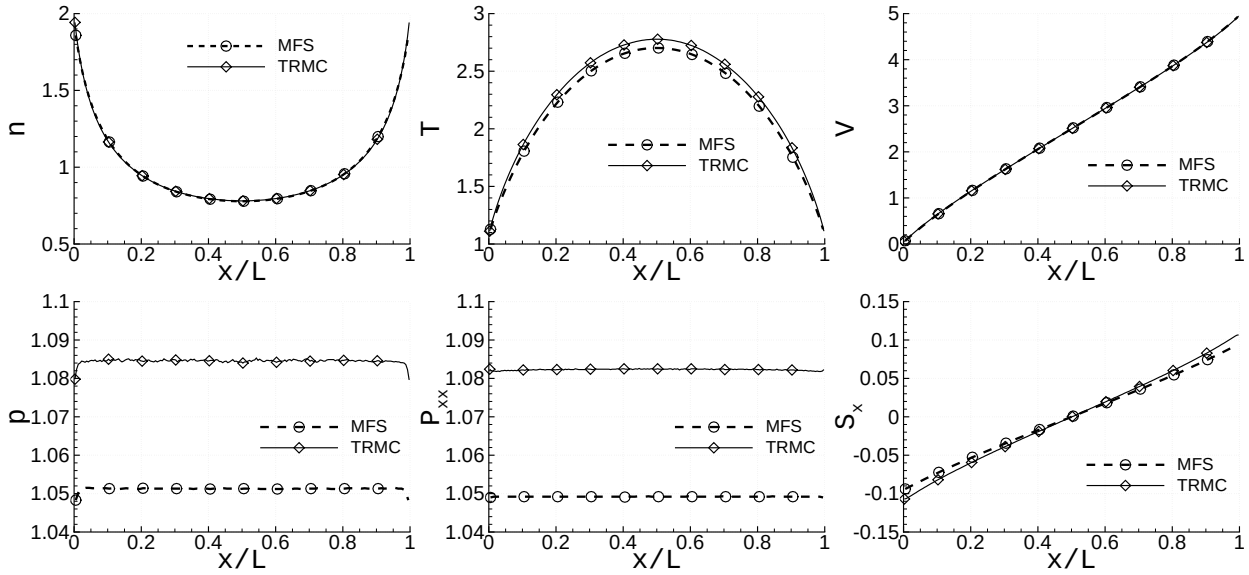

FIGURE 3. Knudsen number Kn = 0.01, plate velocity $S = 5$

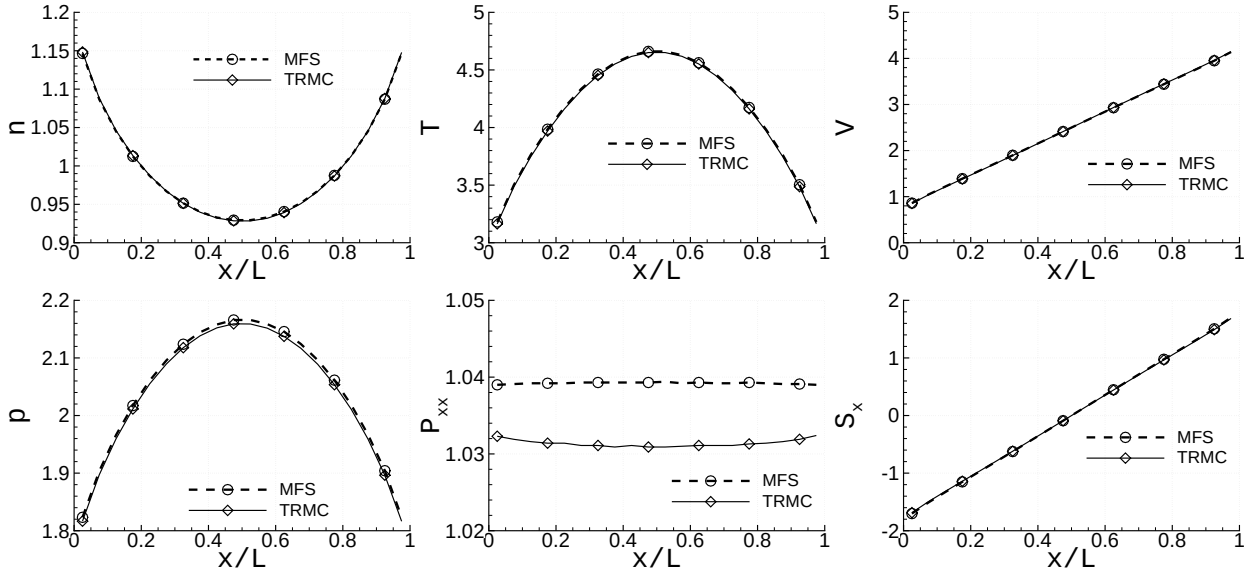

FIGURE 4. Knudsen number Kn = 1, plate velocity $S = 5$

Results of the simulation are shown in Figs. 1, 2, 3, and 4. There are profiles of density, temperature, velocity of the gas and pressure, shear stress tensor component P_{xx}, and heat-flux component S_x. All the results in the figures are presented in dimensionless form. The density is scaled by n_0, the temperature is scaled by T_w, and the gas velocity is scaled by V_t. The pressure p and the stress P_{xx} are scaled by $n_0 m V_t^2$, and the heat-flux component S_x is scaled by $n_0 m V_t^3$. The time step in all cases was relatively small: $\Delta t = 0.1\Delta x/\sqrt{2RT_1}$.

The results for Case 1 are shown in Figure 1. There occurs gas heating in channel, so there is a peak in the gas-temperature profile and a minimum in the density at the middle point of the channel ($X/L = 0.5$). For Case 1, the pressure is very close to a constant value across the channel (note that the continuum approach for the Couette flow provides a constant value of pressure). The momentum conservation equations imply that the value of the stress component P_{xx} is constant. Hence, the value of P_{xx} and its constancy across the channel are the good criteria for

validation of new schemes (see the P_{xx} profiles). For Case 1, the heat flux due to changes in temperature in the channel is quite small. It is seen that the profiles of the x component of the heat flux for the TRMC and MFS schemes are fairly close. Note that excellent coincidence of the simulations results for the MFS and TRMC schemes was obtained for this case.

The results for Case 2 are shown in Figure 2. For such a flow (Knudsen number $\mathrm{Kn} = 1$), the gas pressure is not constant across the channel, which is associated with a nonequilibrium velocity-distribution function. We can see that the value of P_{xx} is constant across the channel. In Case 2, we obtain quite good coincidence of the simulations results for the MFS and TRMC schemes.

In Figures 3 and 4, the results for cases of a higher wall velocity ($S = 5$) are presented. For Case 3 (Fig. 3, $\mathrm{Kn} = 0.01$), the gas pressure near the walls (in the Knudsen layers) becomes slightly lower. Both schemes reproduce this effect. The mean pressure in the channel outside the Knudsen layers in the TRMC scheme, however, is 3% higher than that in the MFS scheme. Both schemes reproduce the constant value of P_{xx}. There is a small difference between the profiles of the heat-flux component S_x. Figure 4 for Case 4 ($\mathrm{Kn} = 1, S = 5$) shows that there is good accordance between TRMC and MFS in terms of density, temperature, pressure, and heat flux S_x. There is a little difference (less than 1%) in P_{xx} values for the MFS and TRMC schemes. The TRMC scheme produces a small bowl in the P_{xx} profile. However, the bowl is very small (about 0.1%), so the results obtained by the TRMC scheme are acceptable for this case.

CONCLUSIONS

The applicability of the Time-Relaxed Monte Carlo method for simulating rarefied gas flows is analyzed by comparisons with the DSMC method. The comparison shows that the TRMC scheme yields results close to the DSMC method for a plane Couette flow for Knudsen numbers 1 and 0.01 and dimensionless wall velocity 1 and 5. The results obtained show that the density, temperature, and velocity profiles coincide for both schemes in all cases. There is a noticeable difference only in the profiles of the shear stress tensor component P_{xx} for cases with the higher value of dimensionless wall velocity $S = 5$ (the difference does not exceed 1%). A possible reason for the difference in results is a high sensitivity of the TRMC schemes to the magnitude of the time step. This issue requires additional investigations. It is also planned to perform a comparison between MFS and recently developed Recursive-TRMC schemes [10], which are based on the whole Wild sum expansion of the solution, and therefore are *exact* in time.

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